

Perfluorododecanoic acid
307-55-1 | DTXSID8031861

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 83.1

Global applicability domain: Outside

Local applicability domain index: 1.38e-01

Confidence level: 4.62e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1'-Isopropylidenebis(4-(1,1,2,2-tetrafluoroethoxy)benzene)</div> <div>Measured: 22400</div> <div>Predicted: 356</div>	<div>Image not found</div> <div>Tris(2,3-dibromopropyl)phosphate</div> <div>Measured: 3.24</div> <div>Predicted: 5.93</div>	<div>Image not found</div> <div>Bis(2-ethylhexyl) phosphate</div> <div>Measured: 4.37</div> <div>Predicted: 5.58</div>
<div>Image not found</div> <div>Triphenyl phosphate</div> <div>Measured: 191</div> <div>Predicted: 4.04</div>	<div>Image not found</div> <div>Flutolanil</div> <div>Measured: 19.5</div> <div>Predicted: 4.67</div>	